Can stable and accurate neural networks always be computed?

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Joint work with: Vegard Antun (Oslo), Anders Hansen (Cambridge)

Based on: M. Colbrook, V. Antun, A. Hansen, "Can stable and accurate neural networks be computed? - On the barriers of deep learning and Smale's 18th problem"

Code: www.github.com/Comp-Foundations-and-Barriers-of-AI/firenet

Interest in deep learning unprecedented and exponentially growing

Machine Learning Arxiv Papers per Year

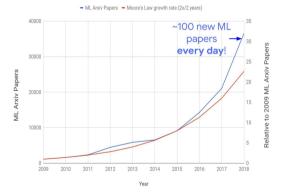
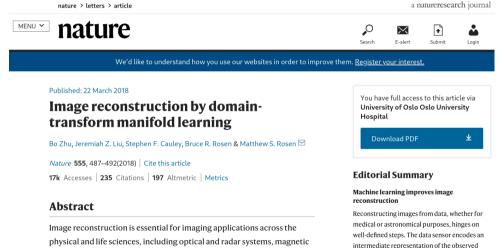


Figure: Source: 'Deep Learning to Solve Challenging Problems' (Google AI) To keep up last year, you would need to continually read a paper every < 5 mins!

Will AI replace standard algorithms in medical imaging?

"superior immunity to noise and a reduction in reconstruction artefacts compared with conventional handcrafted reconstruction methods"

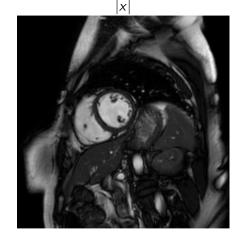


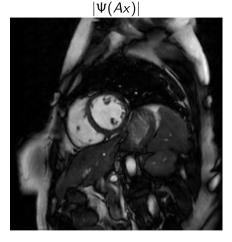
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physical and life sciences, including optical and radar systems, magnetic resonance imaging, X-ray computed tomography, positron emission tomography, ultrasound imaging and radio astronomy^{1,2,3}. During image

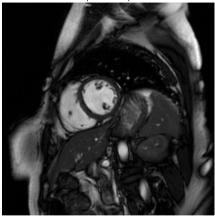
DL is unstable in inverse problems!

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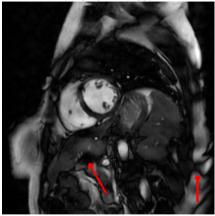




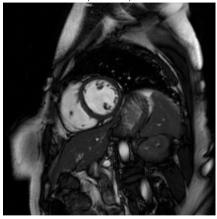
 $|x + r_1|$



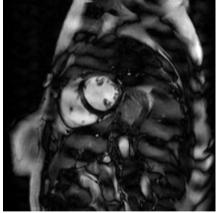
$$|\Psi(A(x+r_1))|$$



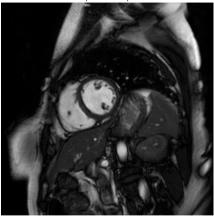
$$|x + r_2|$$



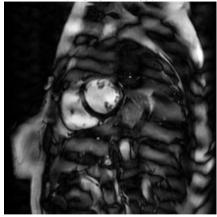
$$|\Psi(A(x+r_2))|$$



$$|x + r_3|$$

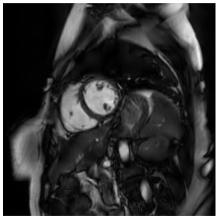


$$|\Psi(A(x+r_3))|$$

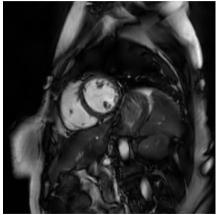


Reconstruction using state-of-the-art standard methods

SoA from Ax



SoA from $A(x + r_3)$



Facebook and NYU's 2020 FastMRI challenge

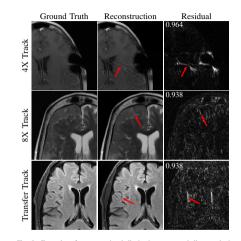


Fig. 6. Examples of reconstruction hallucinations among challenge submissions with SSIM scores over residual plots (residuals magnified by 5). (*top*) A 4X submission from Neurospin generated a false vessel, possibly related to susceptibilities introduced by surgical staples. (*niiddle*) An 8X submission from ATB introduced a linear bright signal mimicking a cleft of cerebrospinal fluid, as well as blurring of the boundaries of the extra-axial mass. (*bottom*) A submission from ResoNNance introduced a false sulcus or prominent vessel.

A program for the foundations of DL and AI

Smale's 18th problem*: What are the limits of artificial intelligence?

A program determining the foundations/limitations of deep learning and AI is needed:

- Boundaries of methodologies.
- Universal/intrinsic boundaries (e.g. no algorithm can do it).

There is a key difference between existence and construction here.

Need to also incorporate two pillars of numerical analysis:

- Stability
- Accuracy

GOAL for rest of talk: Develop some results in this direction for inverse problems.

*Steve Smale composed a list of problems for the 21st century in reply to a request of Vladimir Arnold inspired by Hilbert's list.

Mathematical setup

Given measurements y = Ax + e recover $x \in \mathbb{C}^N$.

- ▶ $x \in \mathbb{C}^N$ be an unknown vector,
- ▶ $A \in \mathbb{C}^{m \times N}$ be a matrix (m < N) describing modality (e.g. MRI), and

•
$$y = Ax + e$$
 the noisy measurements of x.

Outline:

- Fundamental barriers
- Sufficient conditions and Fast Iterative REstarted NETworks (FIRENETs)
- Balancing stability and accuracy

Can we compute neural networks that solve (P_j) ?

Sparse regularisation (benchmark method):

$$\begin{split} \min_{x \in \mathbb{C}^{N}} \|x\|_{l^{1}} & \text{subject to} \quad \|Ax - y\|_{l^{2}} \leq \eta \\ & \min_{x \in \mathbb{C}^{N}} \lambda \|x\|_{l^{1}} + \|Ax - y\|_{l^{2}}^{2} \\ & \min_{x \in \mathbb{C}^{N}} \lambda \|x\|_{l^{1}} + \|Ax - y\|_{l^{2}} \end{split} \tag{P_{2}}$$

Denote the **minimising** vectors by Ξ .

- > Avoid bizarre, unnatural & pathological mappings: (P_j) well-understood & well-used!
- Simpler solution map than inverse problem \Rightarrow stronger impossibility results.
- > DL has also been used to speed up sparse regularisation and tackle (P_j) .

The set-up

$$A \in \mathbb{C}^{m imes N}$$
 (modality), $S = \{y_k\}_{k=1}^R \subset \mathbb{C}^m$ (samples), $R < \infty$

Question: Given a collection Ω of (A, S), does there <u>exist</u> a neural network approximating Ξ (solution map of (P_j)), and <u>can it be trained</u> by an algorithm?

In practice, the matrix A is not known exactly or cannot be stored to infinite precision.

Assume access to: $\{y_{k,n}\}_{k=1}^R$ and A_n (rational approximations, e.g. floats) such that $\|y_{k,n} - y_k\| \le 2^{-n}, \quad \|A_n - A\| \le 2^{-n}, \quad \forall n \in \mathbb{N}.$ And $\{x_{k,n}\}_{k=1}^R$ such that $\inf_{x^* \in \Xi(A_n, y_{k,n})} \|x_{k,n} - x^*\| \le 2^{-n}, \quad \forall n \in \mathbb{N}.$

Training set associated with $(\mathcal{A},\mathcal{S})\in\Omega$ is

$$\iota_{\mathcal{A},\mathcal{S}} \coloneqq \{ (y_{k,n}, \mathcal{A}_n, x_{k,n}) \mid k = 1, \dots, R, \text{ and } n \in \mathbb{N} \}.$$

$$\min_{x \in \mathbb{C}^{N}} \|x\|_{l^{1}} \text{ subject to } \|Ax - y\|_{l^{2}} \leq \eta$$

$$\min_{x \in \mathbb{C}^{N}} \lambda \|x\|_{l^{1}} + \|Ax - y\|_{l^{2}}^{2}$$

$$\min_{x \in \mathbb{C}^{N}} \lambda \|x\|_{l^{1}} + \|Ax - y\|_{l^{2}}$$

$$(P_{2})$$

$$(P_{3})$$

(i) There does not exist a neural network that approximates the function we are interested in.

(ii)

(iii)

$$\min_{x \in \mathbb{C}^{N}} \|x\|_{l^{1}} \text{ subject to } \|Ax - y\|_{l^{2}} \leq \eta$$

$$\min_{x \in \mathbb{C}^{N}} \lambda \|x\|_{l^{1}} + \|Ax - y\|_{l^{2}}^{2}$$

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$$\min_{x \in \mathbb{C}^{N}} \lambda \|x\|_{l^{1}} + \|Ax - y\|_{l^{2}}$$

$$(P_{2})$$

$$(P_{3})$$

- (i) There does not exist a neural network that approximates the function we are interested in.
- (ii) There does exist a neural network that approximates the function, however, there does not exist an algorithm that can construct the neural network.

(iii)

$$\min_{x \in \mathbb{C}^{N}} \|x\|_{l^{1}} \quad \text{subject to} \quad \|Ax - y\|_{l^{2}} \leq \eta$$

$$\min_{x \in \mathbb{C}^{N}} \lambda \|x\|_{l^{1}} + \|Ax - y\|_{l^{2}}^{2}$$

$$\min_{x \in \mathbb{C}^{N}} \lambda \|x\|_{l^{1}} + \|Ax - y\|_{l^{2}}$$

$$(P_{2})$$

$$(P_{3})$$

- (i) There does not exist a neural network that approximates the function we are interested in.
- (ii) There does exist a neural network that approximates the function, however, there does not exist an algorithm that can construct the neural network.
- (iii) There does exist a neural network that approximates the function, and an algorithm to construct it. However, the algorithm will need prohibitively many samples.

Bad news - can't necessarily approximate such a neural network

Theorem

For (P_j) , $N \ge 2$ and m < N. Let K > 2 be a positive integer, $L \in \mathbb{N}$. Then there exists a well-conditioned class (condition numbers ≤ 1) Ω of elements (A, S) s.t. (Ω fixed in what follows):

(i) There does not exist any algorithm that, given a training set $\iota_{A,S}$, produces a neural network $\phi_{A,S}$ with

$$\min_{y\in\mathcal{S}}\inf_{x^*\in\Xi(A,y)}\|\phi_{A,\mathcal{S}}(y)-x^*\|_{l^2}\leq 10^{-\kappa},\quad\forall\,(A,\mathcal{S})\in\Omega.$$
(1)

Furthermore, for any p > 1/2, no probabilistic algorithm can produce a neural network $\phi_{A,S}$ such that (1) holds with probability at least p.

(ii) There exists an algorithm that produces a neural network $\phi_{A,S}$ such that

$$\max_{y\in\mathcal{S}}\inf_{x^*\in\Xi(A,y)}\|\phi_{A,\mathcal{S}}(y)-x^*\|_{l^2}\leq 10^{-(\mathcal{K}-1)},\quad\forall\,(A,\mathcal{S})\in\Omega.$$

However, for any such algorithm (even probabilistic), $M \in \mathbb{N}$ and $p \in \left[0, \frac{N-m}{N+1-m}\right)$, there exists a training set $\iota_{A,S}$ such that for all $y \in S$,

$$\mathbb{P}\Big(\inf_{x^*\in \Xi(A,y)} \|\phi_{A,\mathcal{S}}(y) - x^*\|_{l^2} > 10^{1-\kappa} \text{ or size of training data needed} > M\Big) > p.$$

(iii) There exists an algorithm using only L training data from each $\iota_{A,S}$ that produces a neural network $\phi_{A,S}(y)$ such that

$$\max_{y\in\mathcal{S}}\inf_{x^*\in\Xi(A,y)}\|\phi_{A,\mathcal{S}}(y)-x^*\|_{l^2}\leq 10^{-(K-2)},\quad\forall\,(A,\mathcal{S})\in\Omega.$$

In words...

Nice classes $\boldsymbol{\Omega}$ where one can prove NNs with great approximation qualities exist. But:

- No algorithm, even randomised can train (or compute) such a NN accurate to K digits with probability greater than 1/2.
- There exists a deterministic algorithm that computes a NN with K-1 correct digits, but any such (even randomised) algorithm needs arbitrarily many training data.
- ► There exists a deterministic algorithm that computes a NN with K 2 correct digits using no more than L training samples.

Result independent of neural network architecture - a universal barrier.

Existence vs computation (universal approximation/interpolation theorems not enough).

Conclusion: Theorems on existence of neural networks may have little to do with the neural networks produced in practice.

Numerical example: fails with training methods

dist($\Psi_{A_n}(y_n), \Xi_3(A, y)$)	$dist(\Phi_{A_n}(y_n), \Xi_3(A, y))$	$ A_n - A \le 2^{-n}$ $ y_n - y _{l^2} \le 2^{-n}$	10 ^{-K}	Ω_K
0.2999690	0.2597827	n = 10	10^{-1}	K = 1
0.3000000	0.2598050	n = 20	10^{-1}	K = 1
0.3000000	0.2598052	<i>n</i> = 30	10^{-1}	K = 1
0.0030000	0.0025980	n = 10	10 ⁻³	<i>K</i> = 3
0.0030000	0.0025980	n = 20	10^{-3}	<i>K</i> = 3
0.0030000	0.0025980	n = 30	10^{-3}	<i>K</i> = 3
0.000030	0.0000015	n = 10	10^{-6}	K = 6
0.000030	0.0000015	n = 20	10^{-6}	K = 6
0.000030	0.0000015	<i>n</i> = 30	10^{-6}	K = 6

Table: (Impossibility of computing the existing neural network to arbitary accuracy). A constructed from discrete cosine transform, R = 8000, N = 20, m = 19, solutions are 6-sparse. We demonstrate the impossibility statement (i) on FIRENETs Φ_{A_n} , and LISTA (learned iterative shrinkage thresholding algorithm) networks Ψ_{A_n} . The table shows the shortest l^2 distance between the output from the networks, and the true minimizer of the problem (P_3), with $w_l = 1$ and $\lambda = 1$, for different values of n and K.

Can we avoid this?

$$\hat{x} = \operatorname{argmin} f(x), \quad f^* = \min f(x)$$

Question: Can we find 'good' input classes where

$$f(x) < f^* + \epsilon \implies \|x - \hat{x}\| \lesssim \epsilon$$

We shall see that the answer is yes!

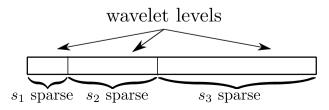
State-of-the-art model for sparse regularisation

Definition [Sparsity in levels]: Let $\mathbf{M} = (M_1, \ldots, M_r) \in \mathbb{N}^r$, where $1 \le M_1 < \cdots < M_r = N$, and $\mathbf{s} = (s_1, \ldots, s_r) \in \mathbb{N}_0^r$, where $s_k \le M_k - M_{k-1}$ for $k = 1, \ldots, r$ and $M_0 = 0$. A vector $x \in \mathbb{C}^N$ is (\mathbf{s}, \mathbf{M}) -sparse in levels if

$$|\text{supp}(x) \cap \{M_{k-1}+1, ..., M_k\}| \le s_k, \quad k = 1, ..., r.$$

The total sparsity is $s = s_1 + ... + s_r$. We denote the set of (s, M)-sparse vectors by $\Sigma_{s,M}$. We also define the following measure of distance of a vector x to $\Sigma_{s,M}$ by

$$\sigma_{\mathbf{s},\mathbf{M}}(x)_{I_{w}^{1}} = \inf\{\|x-z\|_{I_{w}^{1}} : z \in \Sigma_{\mathbf{s},\mathbf{M}}\}.$$



The robust nullspace property

Definition [weighted rNSP in levels]: Let (\mathbf{s}, \mathbf{M}) be local sparsities and sparsity levels respectively. For weights $\{w_i\}_{i=1}^N$ $(w_i > 0)$, we say that $A \in \mathbb{C}^{m \times N}$ satisfies the weighted robust null space property in levels (weighted rNSPL) of order (\mathbf{s}, \mathbf{M}) with constants $0 < \rho < 1$ and $\gamma > 0$ if for any (\mathbf{s}, \mathbf{M}) support set Δ ,

$$\|x_{\Delta}\|_{l^2} \leq \frac{\rho \|x_{\Delta^c}\|_{l^1_w}}{\sqrt{\xi}} + \gamma \|Ax\|_{l^2}, \qquad \text{for all } x \in \mathbb{C}^N.$$

$$\begin{split} \xi &\coloneqq \sum_{k=1}^{r} w_{(k)}^{2} s_{k}, \quad \zeta \coloneqq \min_{k=1,\dots,r} w_{(k)}^{2} s_{k}, \quad \kappa \coloneqq \frac{\xi}{\zeta}. \\ \text{rNSPL} \Rightarrow \|z_{1} - z_{2}\|_{l^{2}} \lesssim \underbrace{\sigma_{\mathsf{s},\mathsf{M}}(z_{2})_{l_{\mathsf{w}}^{1}} + \|Az_{2} - y\|_{l^{2}}}_{\text{"small"}} \\ &+ \underbrace{\left(\lambda \|z_{1}\|_{l_{\mathsf{w}}^{1}} + \|Az_{1} - y\|_{l^{2}} - \lambda \|z_{2}\|_{l_{\mathsf{w}}^{1}} - \|Az_{2} - y\|_{l^{2}}\right)}_{F_{3}^{A}(z_{1},y,\lambda) - F_{3}^{A}(z_{2},y,\lambda)}, \end{split}$$

Main result

Simplified version of Theorem: We provide an algorithm such that:

Input: Sparsity parameters (\mathbf{s}, \mathbf{M}) , weights $\{w_i\}_{i=1}^N$, $A \in \mathbb{C}^{m \times N}$ (with the input A given by $\{A_l\}$) satisfying the rNSPL with constants $0 < \rho < 1$ and $\gamma > 0$. $n \in \mathbb{N}$ and positive $\{\delta, b_1, b_2\}$.

Output: A neural network ϕ_n with $\mathcal{O}(n)$ layers and the following property.

For any $x \in \mathbb{C}^N$ and $y \in \mathbb{C}^m$ with

$$\underbrace{\sigma_{\mathsf{s},\mathsf{M}}(x)_{I_w^1}}_{\mathsf{H}} + \underbrace{\|Ax - y\|_{I^2}}_{\mathsf{I}} \lesssim \delta, \quad \|x\|_{I^2} \lesssim b_1, \quad \|y\|_{I^2} \lesssim b_2,$$

distance to sparse in levels vectors noise of measurements

we have the following stable and exponential convergence guarantee in n

$$\|\phi_n(y)-x\|_{l^2} \lesssim \delta + e^{-n}.$$

Demonstration of convergence age Fourier Sampling Walsh Sa

Image

Walsh Sampling

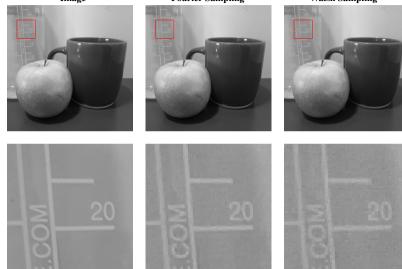
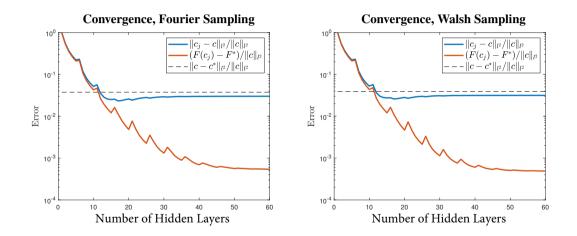
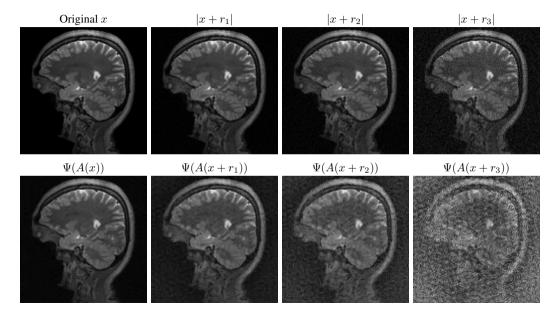


Figure: Images corrupted with 2% Gaussian noise and reconstructed using 15% sampling.

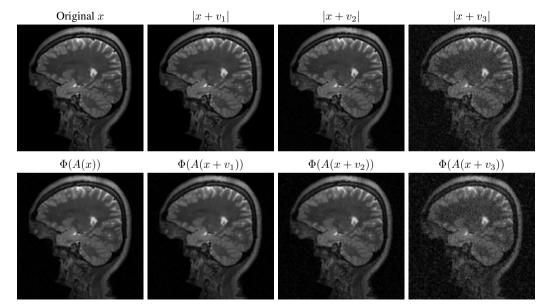
Demonstration of convergence



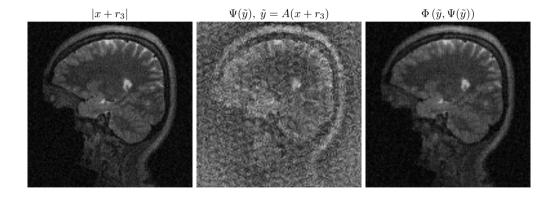
Stable? AUTOMAP X



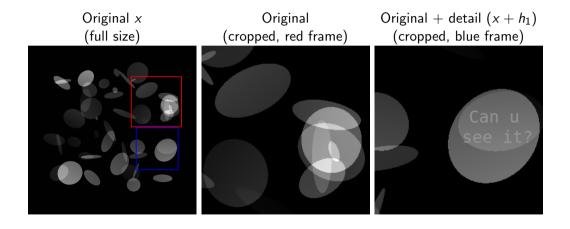
Stable? FIRENETs 🗸



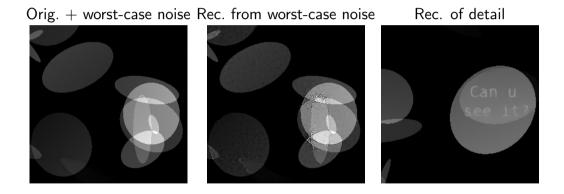
Adding FIRENET layers stabilises AUTOMAP



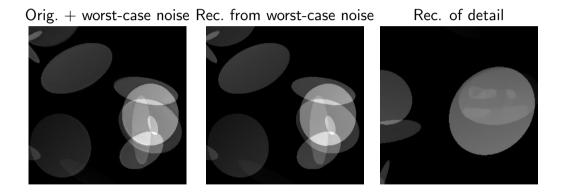
Stability and accuracy, and false negative



U-net trained without noise

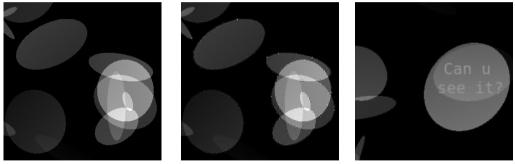


U-net trained with noise



FIRENET

Orig. + worst-case noise Rec. from worst-case noise Rec. of detail



Concluding remarks

There is a need for foundations in AI/deep learning. Our results:

- There are well-conditioned problems where mappings from training data to suitable NNs exist, but no training algorithm (even randomised) can approximate them.
- Existence of algorithms depends on desired accuracy. ∀K ∈ Z≥3, ∃ well-conditioned problems where simultaneously:
 - (i) Algorithms may compute NNs to K-1 digits of accuracy, but not K.
 - (ii) Achieving K 1 digits of accuracy requires arbitrarily many training data.
 - (iii) Achieving K 2 correct digits requires only one training datum.
- Under specific conditions, there are algorithms that compute stable NNs. E.g., Fast Iterative REstarted NETworks (FIRENETs) converge exponentially in the number of hidden layers. We prove FIRENETs withstand adversarial attacks.
- ► There is a trade-off between stability and accuracy in deep learning.

Question: How do we optimally traverse the stability & accuracy trade-off? FIRENETs provide a balance but are likely not the end of the story.

Hopefully this talk has inspired you to build on these results and take up the challenge!